Subject: MATERIALS SCIENCE COLLOQUIUM, Tina M. Nenoff, Sandia National Laboratory, Structure/Property Relationship of Water in Nanoporous Spaces:Characterization of Zeolites, Thursday, May 1, 2008, Building 212, Room A-157, Schlueter, John A
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Date: Thu, 10 Apr 2008 16:42:07 -0500
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MATERIALS SCIENCE COLLOQUIUM

SPEAKER: Tina M. Nenoff
Sandia National Laboratory

TITLE: "Structure/Property Relationship of Water in Nanoporous Spaces: Characterization of Zeolites"

DATE: Thursday, May 1, 2008

TIME: 11:00 a.m.

PLACE: Building 212, Room A-157

HOST: Schlueter, John A

Refreshments will be available at 10:45 a.m

Abstract:

Zeolites and microporous materials are important materials for water purification. Sandia Octahedral Molecular Sieves (SOMS), Na2Nb1.6Ti0.4O5.6(OH)0.4 . H2O, exhibits a high selectivity (105) for divalent cations, which is orders of magnitude better than the sieves end member Na2Nb2O6 . H2O (103). Our research is focused on understanding the effect of the confined water on the ion selectivity in both SOMS frameworks and traditional aluminosilicate Zeolites, like Clinoptilolite ([Ca,Na,K,Li]4-6[Al6(Al,Si)4Si26O72] .24H2O) and silicate clays. Characterization methods used in this study include inelastic neutron scattering (INS), MAS NMR, crystallographic structure refinement, and modeling/simulation. INS and NMR data indicate that the water in Na2Nb1.6Ti0.4O5.6(OH)0.4 . H2O can be described as rotationally free, highly-mobile and bulk-like water species. However, in sharp contrast the occluded water in Na2Nb2O6 . H2O behaves Ice-like and is one of the most rigid water environments investigated in inorganic materials to date. Preliminary DFT calculations of Na2Nb1.6Ti0.4O5.6(OH)0.4 . H2O supports the INS and NMR data of rotationally free waters in energetically favorable locations near the framework atoms. The correlation between structure and property of the materials studied will be discussed.

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